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MEMORANDUM FOR PRS (In-House/Contractor Publication)

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FROM: PROI (STINFO)

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Karl Christe (ERC) et al., "Nitrogen Fluoride Chemistry" (abstract)

↳ 55194 (unofficial notification)

(Statement A)

Dr. Carley
55881

ACS Meeting

(20 August 2002, Boston, MA)

Nitrogen Fluoride Chemistry

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The isomerization of trans-N₂F₂ to cis-N₂F₂ going through N₂F⁺AsF₆⁻ is unpredictable, erratic, requires 2 steps, and consumes an equimolar amount of AsF₅. It was found that catalytic amounts of SbF₅ at 30C can achieve this isomerization, but still result in substantial N₂F₂ losses due to N₂F⁺SbF₆⁻ formation. When the reaction is carried out at 60C, surprisingly NF₄⁺SbF₆⁻.nSbF₅ is formed. The crystal structures of N₂F⁺SbF₆⁻ (disordered), N₂F⁺SbF₆⁻ (disordered), N₂F⁺Sb₂F₁₁⁻ (ordered), and NF₄⁺Sb₂F₁₁⁻ were determined and are discussed. AlF₃ was also studied as a catalyst for the N₂F₂ isomerization and was found to be an ideal catalyst resulting in very high conversions of trans-N₂F₂ and high yields of cis-N₂F₂. The AlF₃ can be used repeatedly without loss of activity or N₂F⁺ salt formation. Cis-N₂F₂ forms with SnF₄ at low temperatures a 2:1 salt, (N₂F⁺)₂SnF₆²⁻, that slowly loses N₂F₂ at room temperature to give N₂F⁺SnF₅⁻. The crystal structure of H₃NF⁺CF₃SO₃⁻ was also determined and exhibits a relatively long N-F bond.

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